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Development and Implementation of an Online Chemistry Module to a Large Eddy Simulation Model

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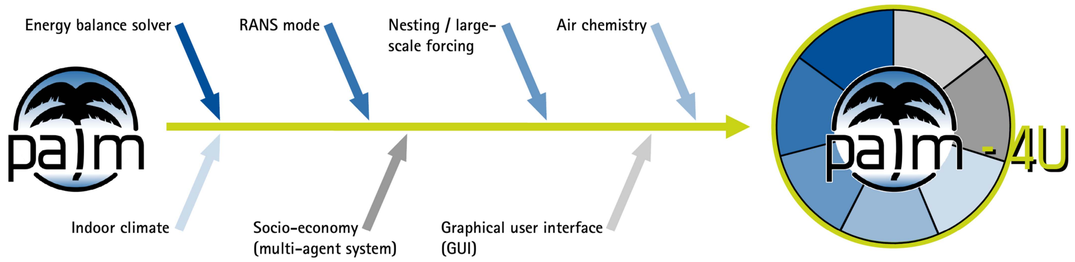
Introduction

Urban climate and air quality have a profound effect on human health, living conditions and quality of life. Adequate modelling tools are required to support urban planning and development strategies for the mitigation of adverse effects on urban climate such as poor air quality. However, a realistic implementation of urban canopy processes still poses a serious challenge for current weather and air quality models due to the small scale of the phenomena to be described.

To address this demand, a new urban climate model (UCM) is developed within the joint project **MOSAIK** (**Mo**dellbasierte **S**tadtplanung und **A**nwendung **i**m **K**limawandel: Model-based city planning and application in climate change) under the lead of the Institute of Meteorology and Climatology at the Leibniz Universität Hannover.

Development of the Urban Climate Model PALM-4U

The new urban climate model PALM-4U is based on the state-of-the-art **Pa**rallelized **L**arge-Eddy Simulation **M**odel (PALM, Maronga et al, 2015). Large-Eddy Simulation (LES) models explicitly resolve relevant scales of turbulent motion, so that these models can capture the inherent unsteadiness of atmospheric turbulence and advection.



Model development work flow within MOSAIK

The final operational version of PALM-4U, which will be distributed by Leibniz Universität Hannover as Open Source software, will have the following features:

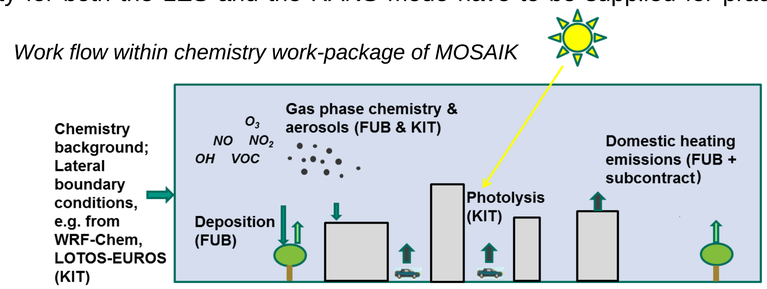
- Magnifying lens function (zoom function) and nesting to large scale models.
- Graphical user interface, NetCDF as Standard I/O data format.
- Scale-dependent turbulence and building parameterizations for resolutions from 1 to 100 m.
- Choice between RANS (Reynolds-Averaged-Navier-Stokes) and LES mode.
- Atmospheric chemistry and air pollution, urban soil water, indoor climate and energy demand.
- Output of human-related quantities (physiological equivalent temperature or universal thermal climate index, also utilizing a multi-agent system).

Implementation of the Chemistry Module

LES models are so far hardly applied for urban air quality studies, in particular when the chemical transformation of pollutants is involved. Due to the high computational demands of an LES based model, compromises in the description of chemical and removal processes are required. Therefore, chemistry modules of different complexity for both the LES and the RANS mode have to be supplied for practical applications.

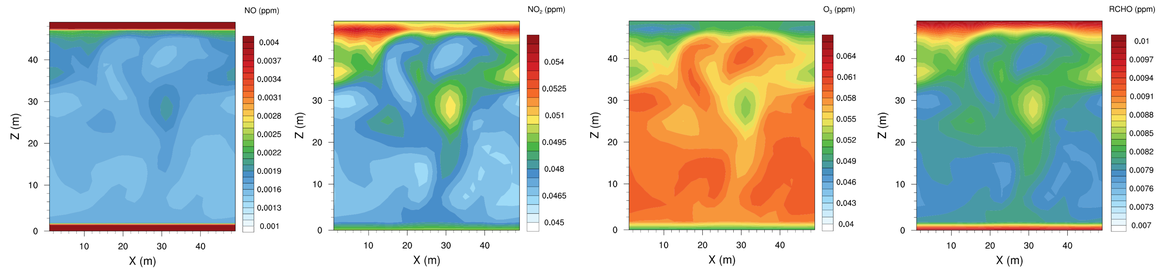
For the RANS mode, the chemistry mechanism is in line with the chemistry schemes suggested within current VDI Guidelines for regulatory purposes in Germany but will be extended by the particle phase (including inorganic and organic aerosols).

Work flow within chemistry work-package of MOSAIK



Gas phase chemistry has been implemented using the Kinetic Preprocessor KPP (Damian et al., 2002) in order to obtain the necessary flexibility in the choice of the chemistry mechanism.

For the LES mode a reduced chemistry mechanism, which includes only major pollutants namely O_3, NO, NO_2, CO, a highly simplified VOC chemistry and a small number of products have been implemented.



Preliminary results show the impact of turbulent structures on simulated pollutant concentration fields. Results based on realistic emissions for an urban environment with explicitly resolved buildings will be presented next year.

References:

MOSAIK web page: https://palm.muk.uni-hannover.de/mosaik/wiki
PALM web page and reference: https://palm.muk.uni-hannover.de/trac
Maronga et al, 2015, Geosci. Model Dev. 8, doi:10.5194/gmd-8-2515-2015
KPP web page: http://people.cs.vt.edu/asandu/Software/Kpp/

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GEFÖRDERT VOM
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